

Procedure for Modeling Complexes

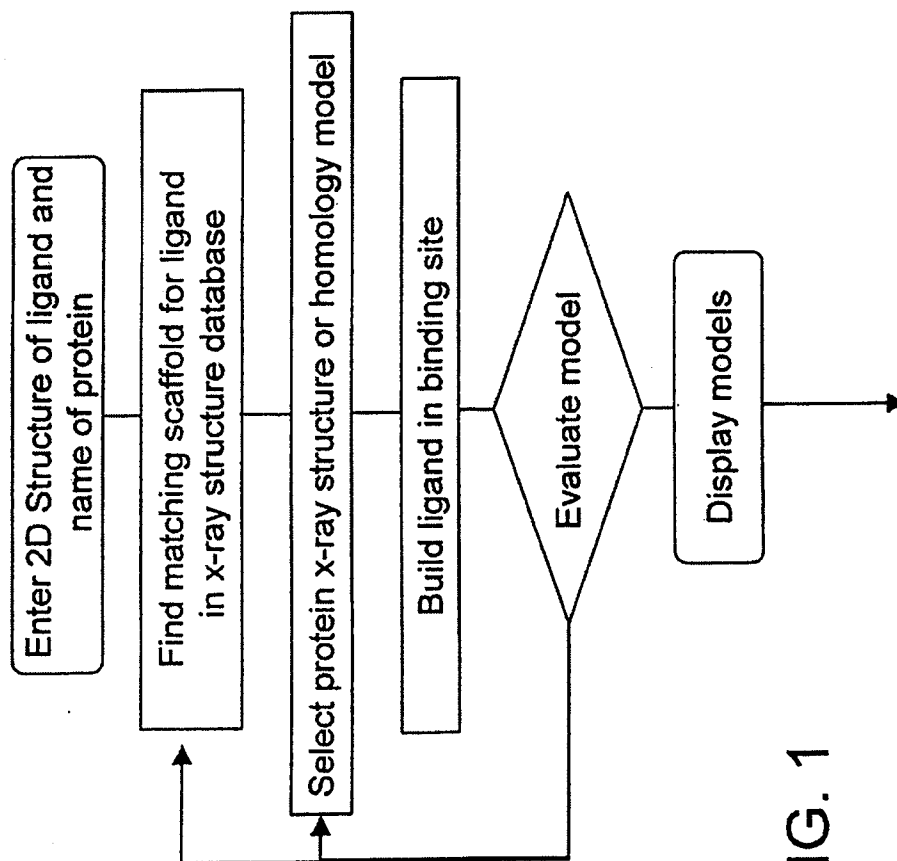
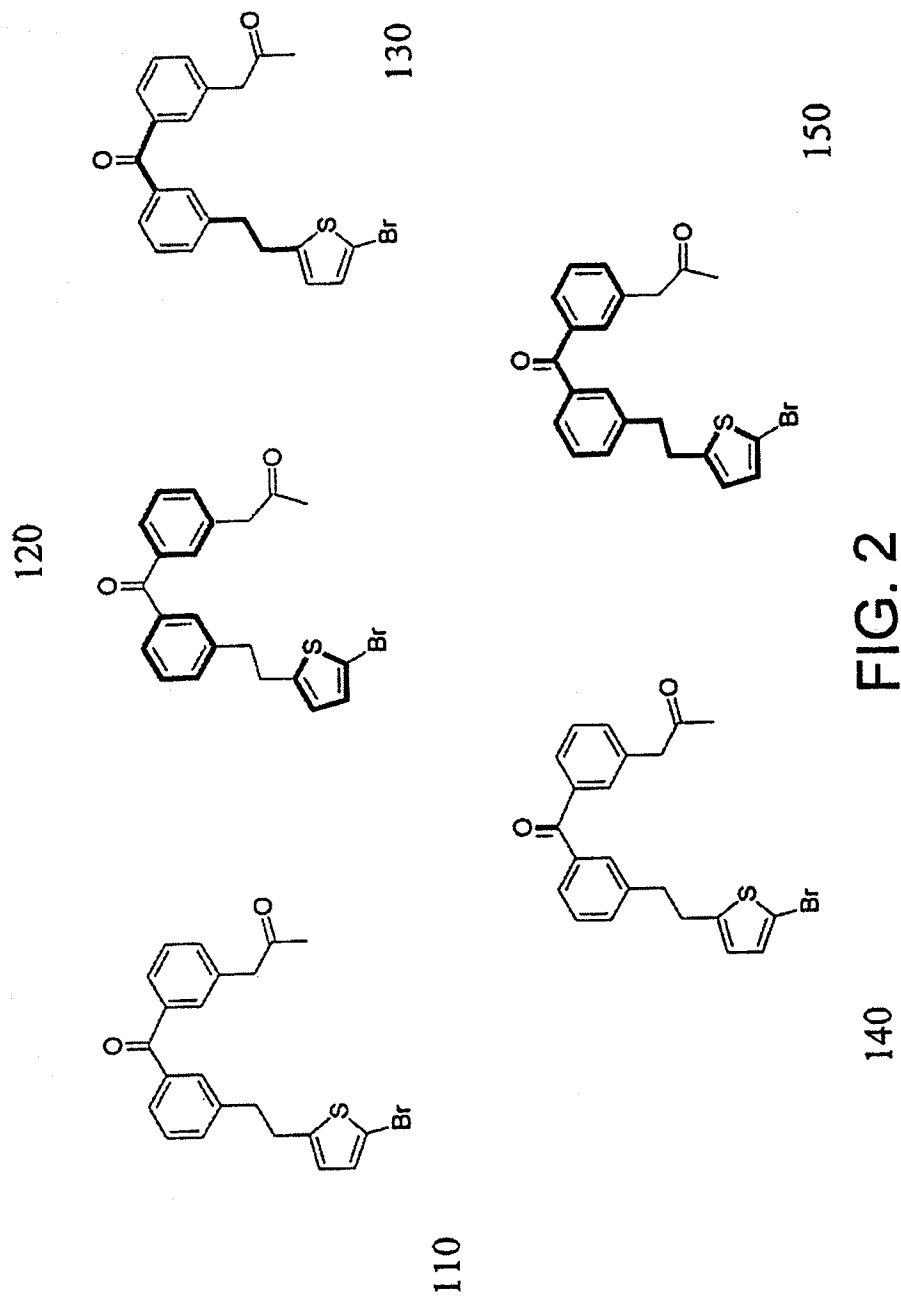


FIG. 1



Maximum Common Substructure

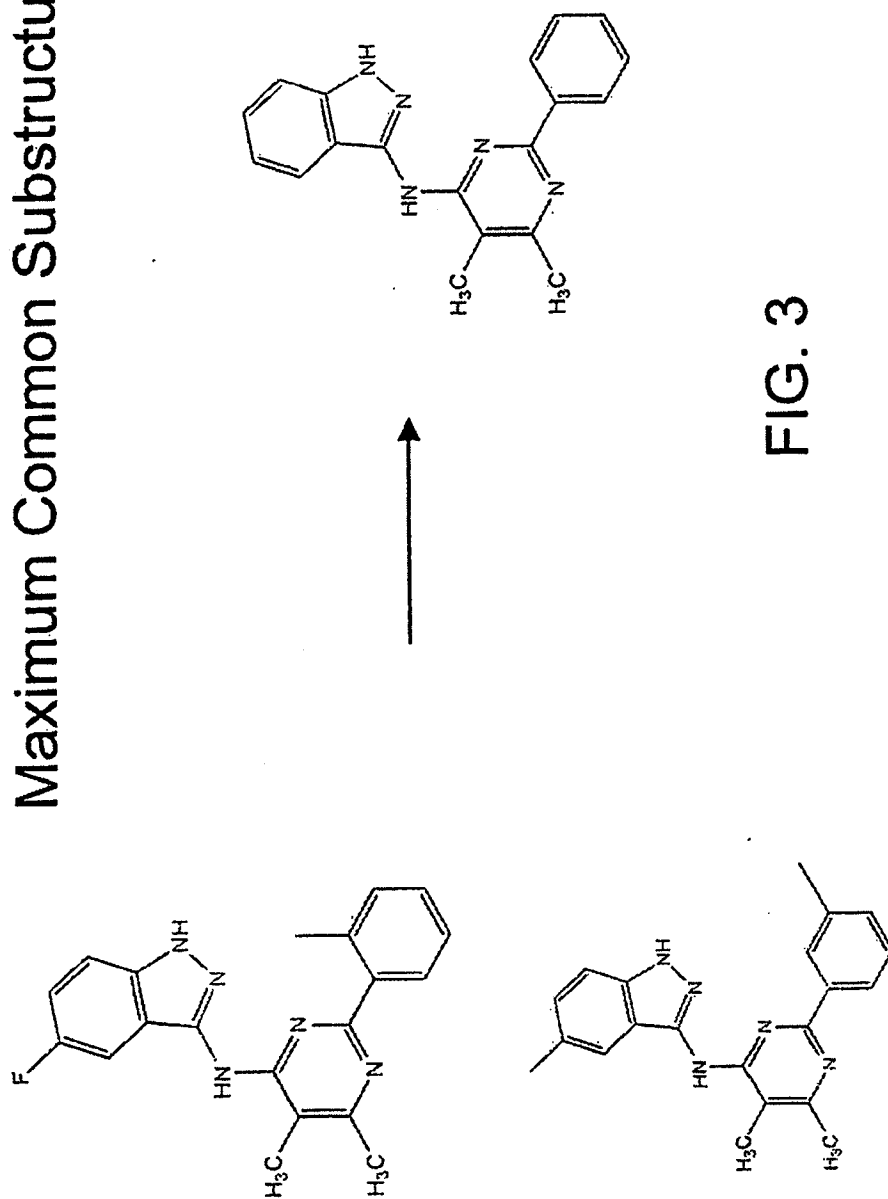


FIG. 3

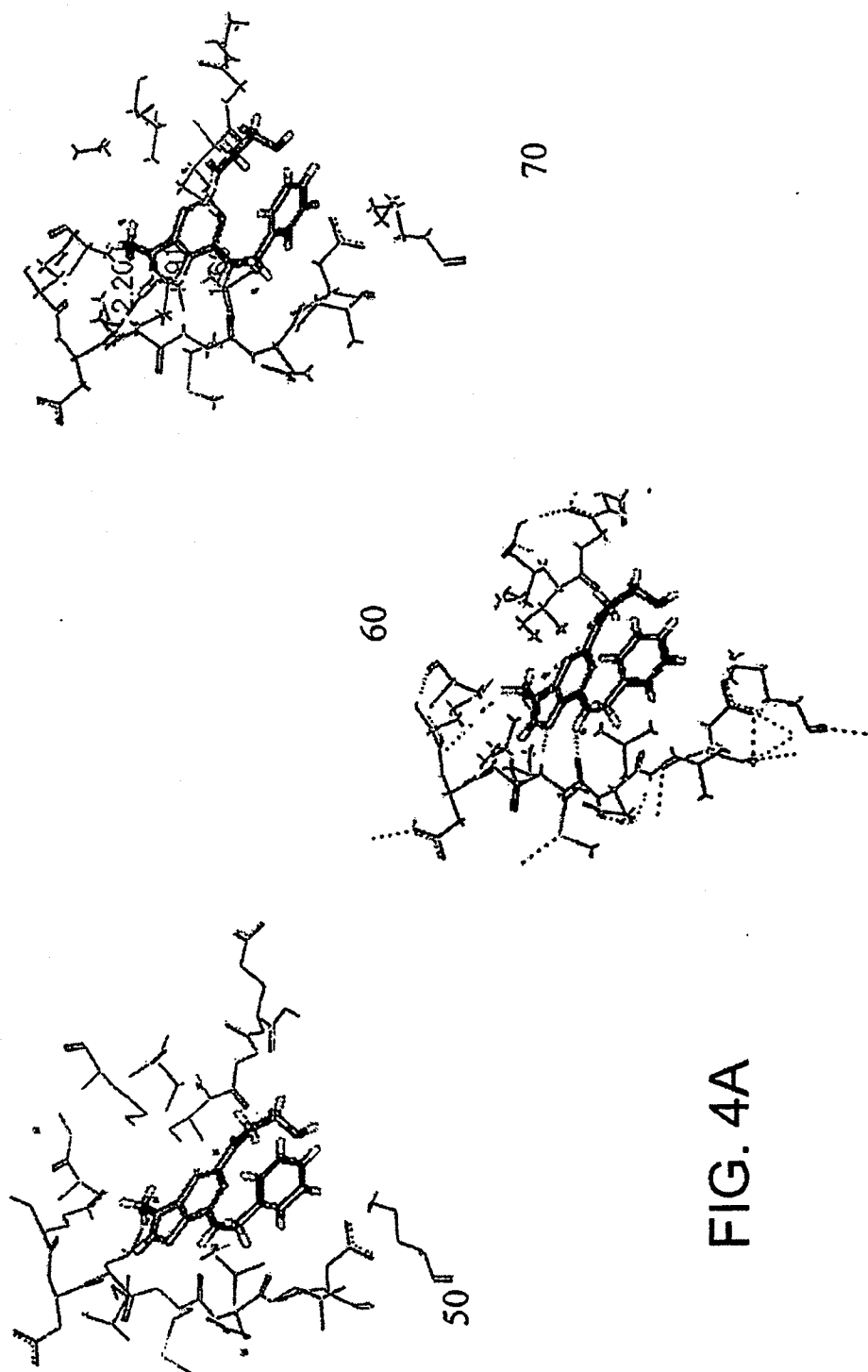
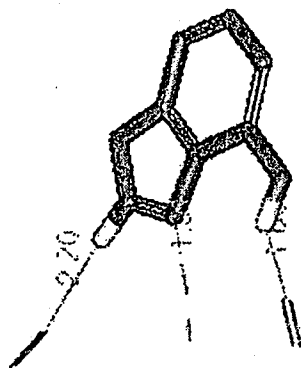
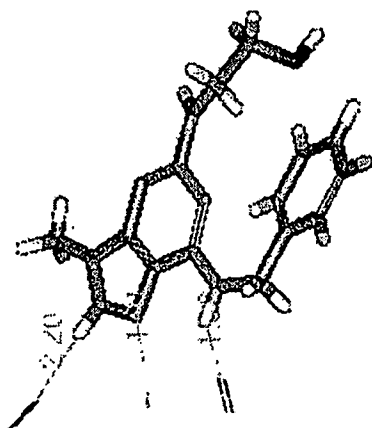


FIG. 4A

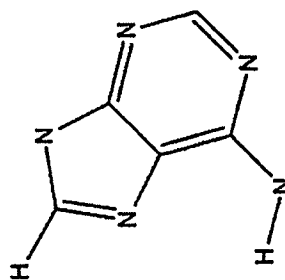


90

FIG. 4B



80



100

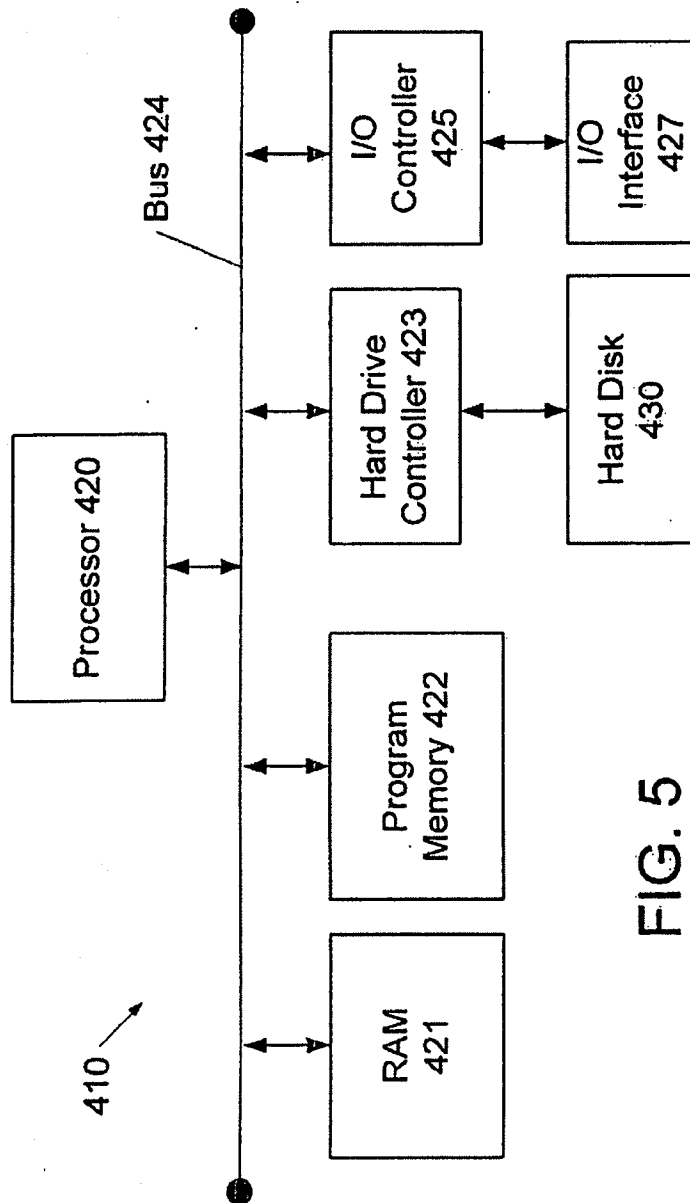


FIG. 5

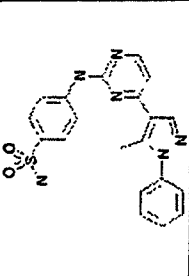
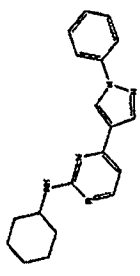
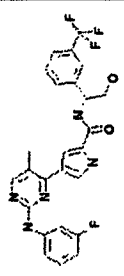
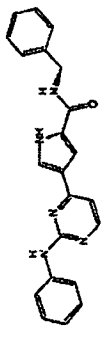
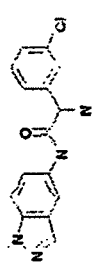
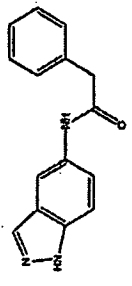
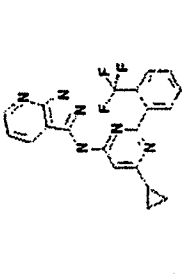
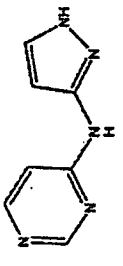
query ligand	protein	scaffold	rmsd (model vs. x-ray) / Angstrom
	jnk3		0.9 – 1.3
	erk2		1.5 – 2.0
	pka(5xm)		1.2
	gsk3β		1.3 – 2.2

FIG. 6

FIG. 7A

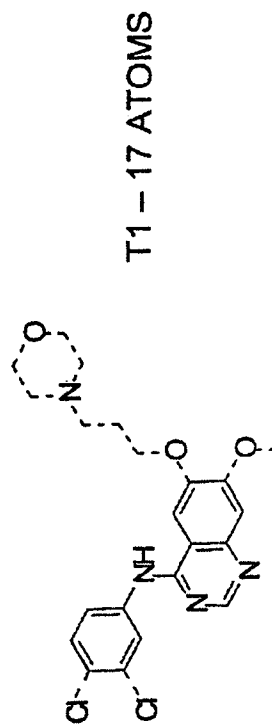


FIG. 7B

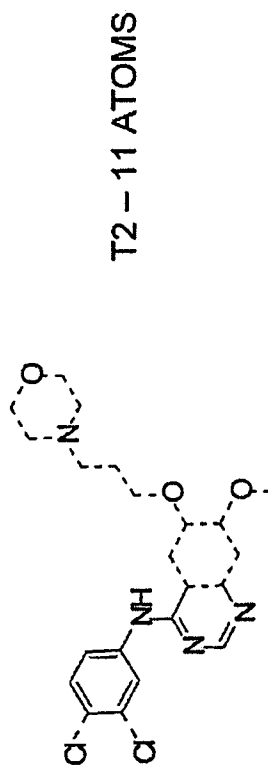
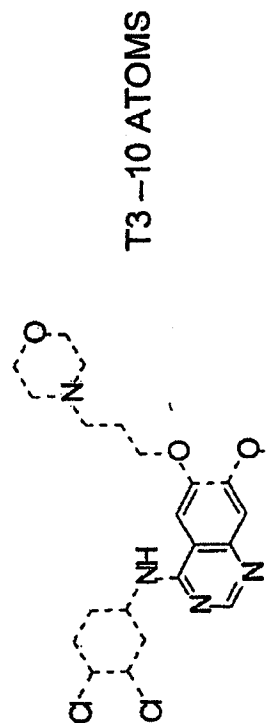


FIG. 7C



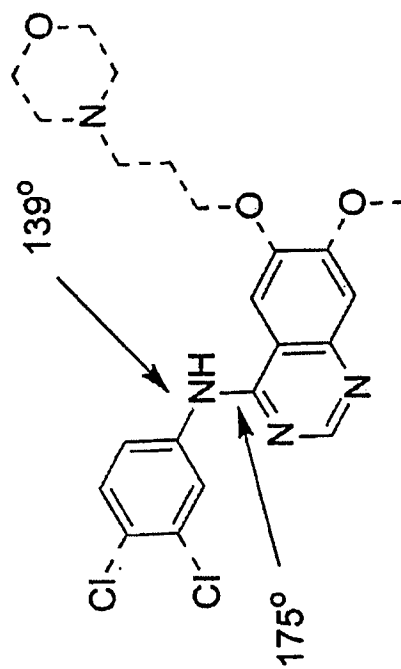


FIG. 8

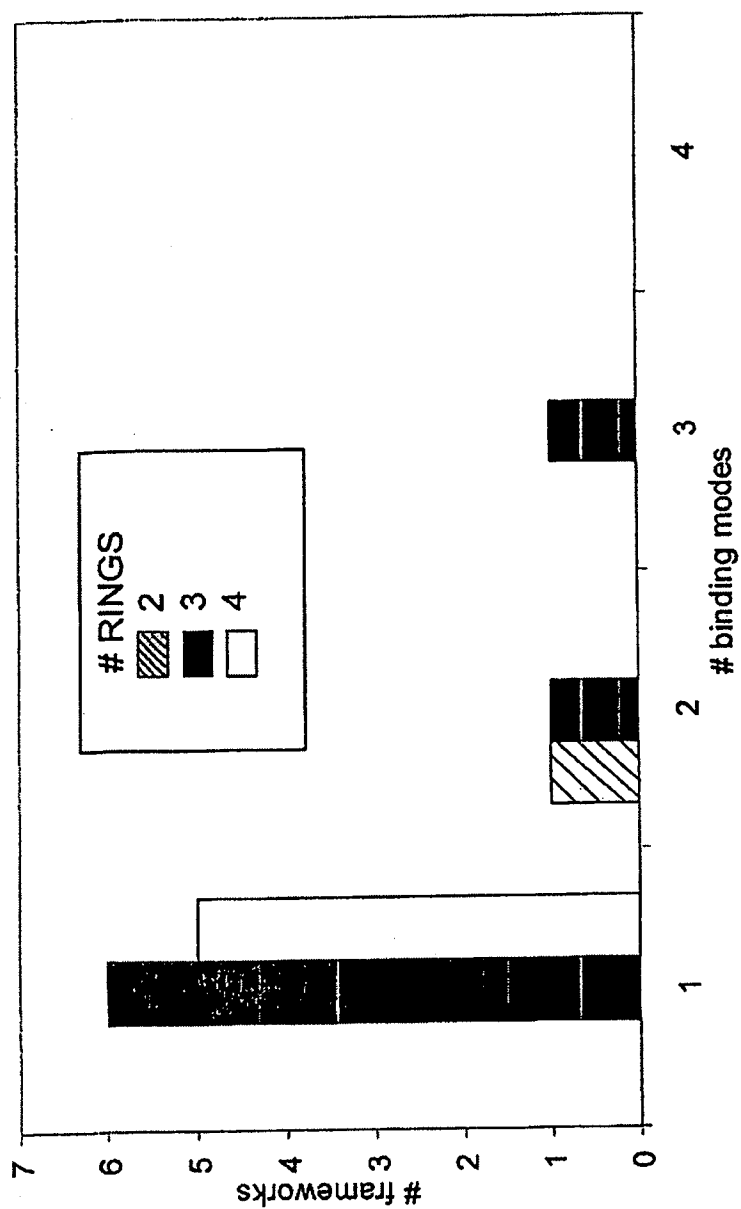


FIG. 9

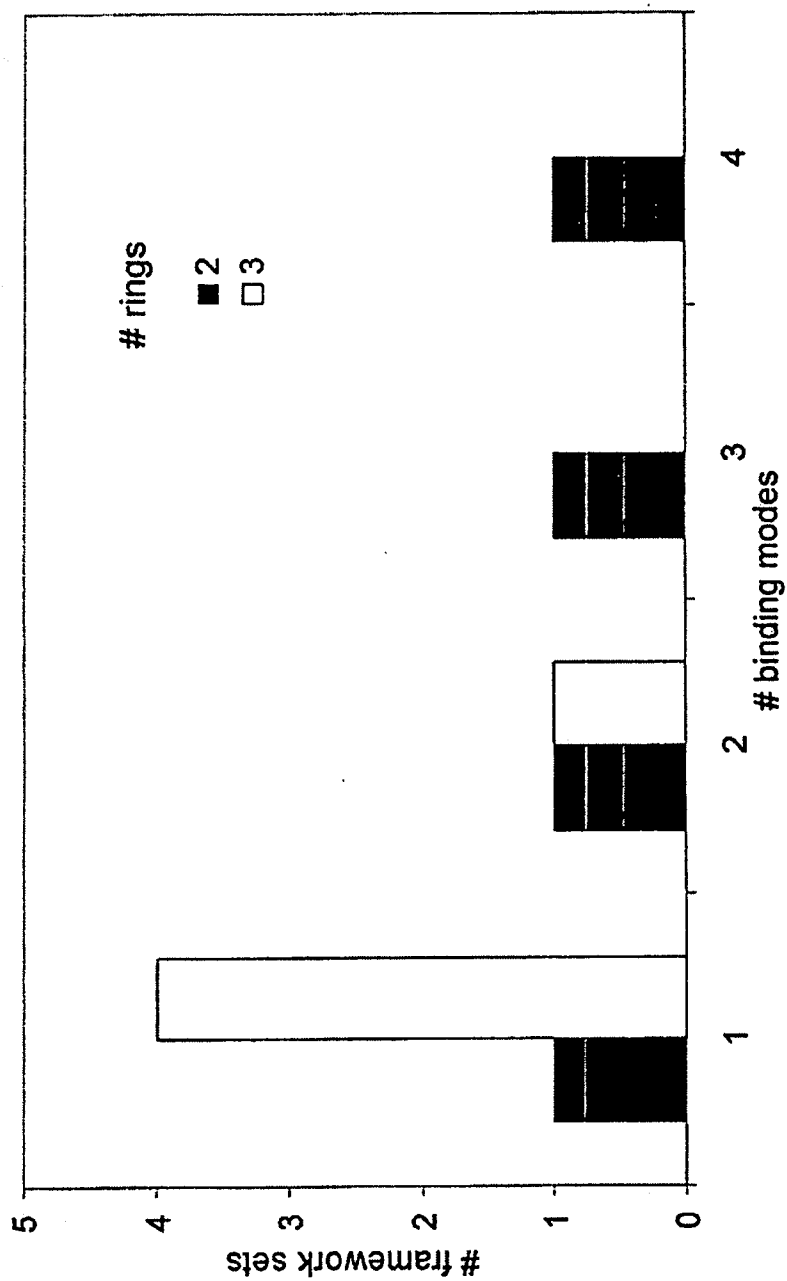


FIG. 10

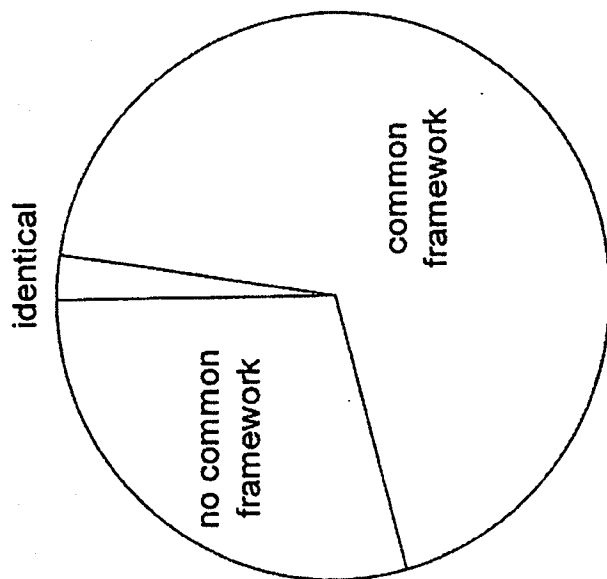


FIG. 11

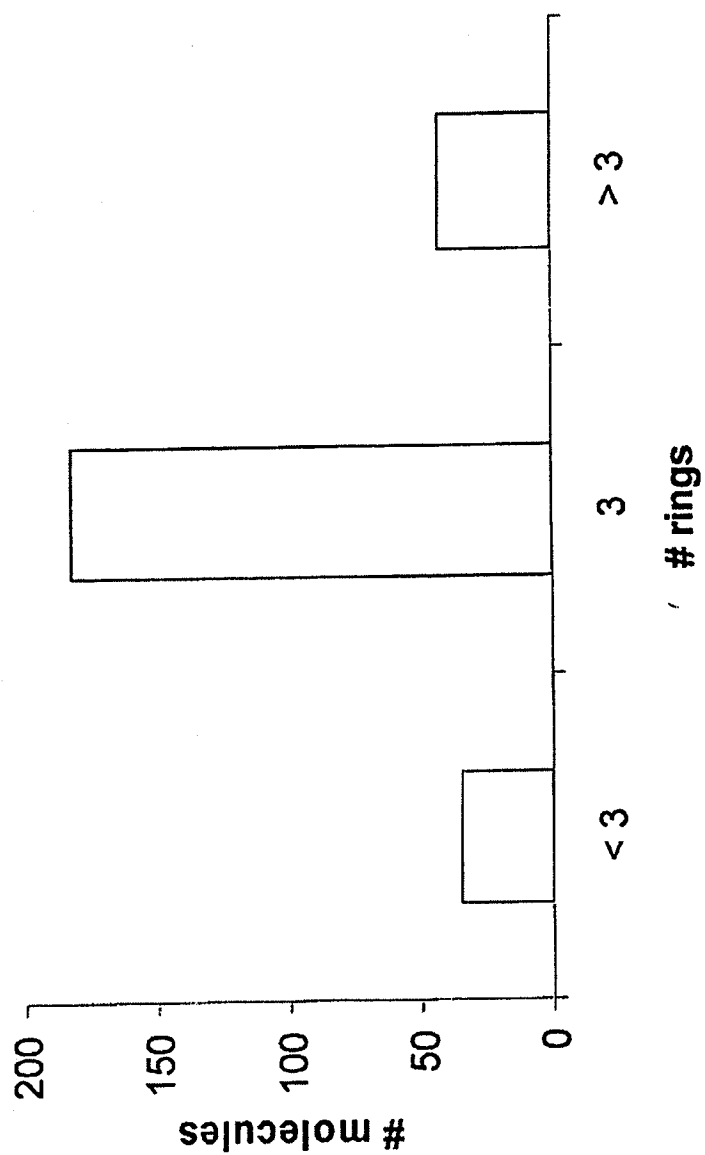
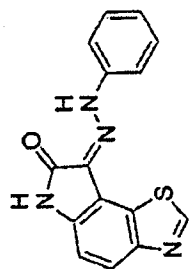
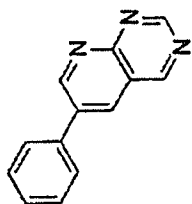


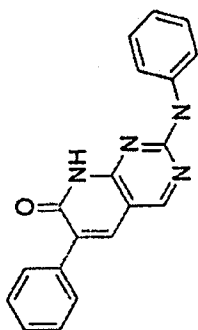
FIG. 12



10



9



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FIG. 13